

Pyrrolidine  
123-75-1 | DTXSID3059559

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -49.9 °C

Global applicability domain: Inside

Local applicability domain index: 5.96e-01

Confidence level: 6.37e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Pyrrolidine</div> <div>Measured: -57.8</div> <div>Predicted: -49.9</div>	<div>Image not found</div> <div>Propyleneimine</div> <div>Measured: -65.0</div> <div>Predicted: -69.4</div>	<div>Image not found</div> <div>Heptamethyleneimine</div> <div>Measured: 29.0</div> <div>Predicted: 15.6</div>
<div>Image not found</div> <div>2-Butanamine, 2-methyl-</div> <div>Measured: -105</div> <div>Predicted: -76.8</div>	<div>Image not found</div> <div>2,5-Dimethylpyrrole</div> <div>Measured: 7.70</div> <div>Predicted: 6.39</div>	